

# The static response and the Local-field factor of the 2-D electron fluid.

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The static local-field factor (LFF) of the interacting 2-D fluid is calculated nonperturbatively using a mapping of the quantum fluid to a classical Coulomb fluid [Phys. Rev. Lett., **87**, 206 (2002)]. The LFF for the paramagnetic fluid *differs markedly* from expectations from standard perturbation theory. Our result for the LFF has a maximum close to  $3k_F$ , while perturbation methods yield a maximum near  $2k_F$ . The available quantum Monte Carlo data seem to agree with our results. These findings imply that many effects, e.g., Friedel oscillations, Kohn anomalies, effective electron-electron interactions, etc., are affected by the strong correlations among anti-parallel spins in 2D.

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*Introduction.* The study of the uniform two-dimensional electron gas (2DEG) continues to bring out new and unexpected properties. Its physics depends crucially on the “coupling parameter”  $\Gamma = (\text{potential energy})/(\text{kinetic energy})$  which defines the strength of the Coulomb interactions. The  $\Gamma$  for the 2DEG at  $T = 0$  and mean density  $n$  turns out to be equal to the mean-disk radius  $r_s = (\pi n)^{-1/2}$  per electron. The density parameter  $r_s$ , the spin polarization  $\zeta$  and the temperature  $T$  are the only physical variables that appear in this problem. As the coupling constant increases, the 2DEG becomes more like a “liquid”, but here we continue to loosely call it an electron “gas”. An important property of the 2DEG which captures many of the exchange and correlation effects and central to its physics is the response function  $\chi(k, \omega)$ . It is expressed in terms of a zeroth-order response  $\chi^0(k, \omega)$  and a local-field factor (LFF), also called a local-field correction (LFC), denoted by  $G(k, \omega)$ .

$$\chi(k, \omega) = \chi(k, \omega)^0 / [1 - V_k(1 - G(k, \omega))] \chi(k, \omega)^0 \quad (1)$$

The LFF is also closely related to the vertex function  $\Lambda(k, \omega)$ . The simplest static form,  $G(k)$ , is identical with  $G(k, 0)$  at  $k = 0$ , and begins to differ from  $G(k, \omega)$  as  $k$  or  $\omega$  increases. In general, the  $G(k, \omega)$  for  $\omega$  smaller than the plasma frequency  $\omega_p$  behaves like a static quantity. Hence the use of a static form  $G(k)$  is often adequate. As such, considerable effort has been devoted to determining  $G(k)$ , using perturbation theory, kinetic equation methods [1, 2], etc. A partially analytic, partially empirical, approach is often implemented by invoking parametrized models constrained to satisfy sum rules [3]. These sum rules invoke physical quantities which are usually obtainable only from numerical simulations. While these efforts have considerably extended the theory beyond the random-phase approximation (RPA) response, its validity is still restricted to the low- $r_s$  regime.

We have shown in a number of recent papers [4, 5, 6] that the static properties of the 2D and 3D electron systems can be calculated *via* an equivalent *classical* Coulomb fluid having a temperature  $T_q$  such that it has

the same correlation energy as the quantum system at the physical temperature  $T = 0$ . The “quantum temperature”  $T_q$  was shown to be given by [6],

$$t = T_q/E_F = 2/[1 + 0.86413(r_s^{1/6} - 1)^2] \quad (2)$$

where  $E_F = 1/r_s^2$  is the Fermi energy in Hartree atomic units. At finite temperatures, the classical-fluid temperature  $T_{cf}$  is taken to be  $(T_q^2 + T^2)^{1/2}$ , as discussed in Ref. [5]. The pair-distribution functions (PDFs) of the classical fluid are calculated using the hyper-netted-chain (HNC) equation [7] inclusive of bridge corrections. A set of three coupled equations, for  $g_{11}$ ,  $g_{12}$  and  $g_{22}$  for the two spin-species  $i=1,2$  is solved. This *classical* mapping of quantum fluids within the HNC was named the CHNC. The static response function and the static structure factor of a classical fluid are identical (except for numerical factors), and we also showed [4, 5] how this can be exploited for a very simple determination of the static LFF of the quantum electron fluid. In ref. [5] we showed that various sum rules, e.g. the behaviour of  $G(k)$  at large  $k$  and its relation to the “on-top” value  $g(0)$  of the pair-distribution function (PDF) are satisfied by this “classically” determined  $G(k)$ , and that the results agreed well with, e.g., the 3D-LFF of Utsumi and Ichimaru [8].

The application of the CHNC method to the 2DEG required the inclusion of short-range clustering effects (“bridge terms”) going beyond the usual HNC approximation. These contributions seem to play a role similar to the “back-flow” contributions used in QMC simulations [9]. Such terms were necessary for  $g_{12}$ , while the need was less stringent for  $g_{11}$  since the Pauli exclusion blocked the clustering for identical spins. However, it is well known that the compressibility sum rule is violated by the HNC approximation, and that a bridge term is in principle necessary [10], even for  $g_{ii}$ . While this shortcoming is not strongly felt in the calculated distribution functions [11], and even less so in the energy, it needs to be addressed if the small- $k$  limit of the LFF is to be correctly recovered.

The objective of this work is to evaluate the LFF of

the 2DEG as a function of  $r_s$  and show that it does *not* behave in the manner expected from standard perturbation calculations [12] using the RPA screened Coulomb interaction. Such calculations give LFFs with a “hump” at  $2k_F$  due to the singular nature of  $\chi(k = 2k_F)$ , while we find that the interactions have moved the hump towards  $\sim 3k_F$ . A limited set of QMC data for the 2-D LFF is available in the literature [13, 14] and seems to be in agreement with our findings. If this is indeed the case, effects like the Kohn anomaly, Friedel oscillations, effective attractive electron-electron interactions [12] etc., would be *weaker* in 2-D. This emphasizes the need for further work in this field.

*The local-field factor.* The LFF was already defined in Eq. 1. Here we are concerned with the static form  $G(k)$ , defined with respect to a reference “zeroth-order” response function. It is customary to use the Lindhard function  $\chi(k)_L^0$  for this purpose. However, a number of authors [15] pointed out that another natural choice is to use the “density-functional” non-interacting form  $\chi(k)^0$  containing the occupation numbers corresponding to the *interacting* density. Richardson and Ashcroft (RA) [16] explicitly constructed a set of LFFs based on this  $\chi(k)^0$ , containing the corrected occupation numbers. The calculation of RA was for the 3DEG, and identified the simplest conserving set of diagrams in the perturbation expansion for the RPA-screened interaction. This set (Fig. 2 of RA) is the same as selected earlier by Geldart and Taylor [17] who calculated the static 3D case. In all cases, dynamic or static, the LFF calculated from the diagrams is further restructured using quantum Monte-Carlo data in several ways. In effect, most of the currently proposed LFFs, be they for 2D (e.g., [13]) or 3D (e.g., [8]), are in some sense only partially analytic since they use the numerical simulation (QMC) data and fit the behaviour at  $k=0$ ,  $k \rightarrow \infty$  and possibly  $S(k)$  etc., to form the LFF. This truly emphasizes the difficulty and delicateness involved in the determination of the LFF.

The CHNC also uses the QMC correlation-energy  $E_c(r_s)$ , at the initial stage of constructing the “quantum temperature”  $T_q(r_s)$  of the classical fluid at zero temperature ( $T = 0$ ). From then on we have a self-contained method for obtaining all the static properties including  $E_c(r_s, \zeta, T)$  and its gradients, as well as  $g(r)$ ,  $S(k)$  etc. The CHNC also provides a *very simple* formula for the LFF, via the classical-fluid LFF. Unlike in the quantum case, for a classical fluid,  $\chi(k)$  is directly related to the structure factor.

$$S_{ij}(k) = -(1/\beta)\chi_{ij}(k)/(n_i n_j)^{1/2} \quad (3)$$

Hence, taking the paramagnetic case for simplicity,

$$V_c(k)G(k) = V_c(k) - \frac{T_{cf}}{n} \left[ \frac{1}{S(k)} - \frac{1}{S^0(k)} \right] \quad (4)$$

Here  $T_{cf}$  equals  $T_q$  if the physical temperature  $T = 0$ . In CHNC, and hence in these expressions, the  $\chi^0(k)$  and  $S^0(k)$  are based on a Slater determinant, while the Lind-

hard function is applicable to the non-interacting case without antisymmetrization of the wavefunction.

The above expressions show that the LFF is immediately available if the interacting and noninteracting structure factors are known. These are explicitly known since the HNC+Bridge equations for the classical fluid yield the PDFs  $g_{ij}(r)$  and Fourier transforms of which directly yield the  $S_{ij}(k)$  needed here. Alternatively, any other source of  $S(k)$ , e.g., QMC, may be used, while  $S^0(k)$  for the 2DEG is analytically known. Equation 4 involves a difference between the inverses of  $S(k)$  and  $S^0(k)$ , and hence it is very desirable to calculate them to the same accuracy, since their difference has to cancel the Coulomb potential which becomes large as  $k \rightarrow 0$ . The Coulomb potential  $V_c(r)$  for point-charge electrons is  $1/r$ . However, the classical electron at the temperature  $T_{cf}$  is localized to within a thermal wavelength. Thus, we use the “diffraction corrected” form [6]

$$V_c(r) = (1/r)[1 - e^{-rk_{th}}] \quad (5)$$

$$V_c(k) = 2\pi[k^{-1} - (k_{th}^2 + k^2)^{-1/2}] \quad (6)$$

The  $k_{th}$  was determined by numerically solving the Schrodinger equation for a pair of 2-D electrons in the potential  $1/r$  and calculating the electron density in each normalized state [18]. It was found that

$$k_{th}/k_{th}^0 = 1.158T_{cf}^{0.103}$$

where  $T_{cf}$  is in a.u., Here  $k_{th}^0$  is the de Broglie thermal wavevector  $(2\pi m^* T_{cf})^{1/2}$ , with  $m^*$ , the reduced mass of the scattering electron-pair, equal to  $1/2$ .

The introduction of the de Broglie wavevector  $k_{th}$  adds a new  $k$ -scale which competes with the Fermi wavevector  $k_F$  of the non-interacting problem. However,  $k_{th}$  becomes equal to about  $k_F$  only when we approach the Wigner crystallization ( $r_s \sim 35$ ) regime. Hence, as far as this study is concerned, the critical wavevector  $k_c$  which separates the small- $k$  region from the large- $k$  region will be taken to be  $2k_F$ . Although Eq. 4 is already very simple to compute, the explicit cancellation of  $V_c$  by the terms in the  $1/S - 1/S_0$  can be realized as follows. For the paramagnetic case, we have:

$$S(k) = 1 + nx[h_{11}(k) + h_{12}(k)] \quad (7)$$

$$= 1/[1 - nx\{c_{11}(k) + c_{12}(k)\}] \quad (8)$$

Here we have used the Orstein-Zernike relations and the direct ( $c_{ij}$ ) and total ( $h_{ij}$ ) correlation functions, while  $x=1/2$  is the fractional composition. The pair-distribution function [6] in CHNC has the form

$$g_{ij}(r) = e^{[-\beta\phi_{ij}(r) - c_{ij}(r) + h_{ij}(r) + B_{ij}(r)]} \quad (9)$$

$$\phi_{ij}(r) = P_{ij}(r)\delta_{ij} + V_c(r) \quad (10)$$

Here  $P_{ij}$  is an effective potential for the Pauli-exclusion effect, and is such that, when used in the HNC equations, reproduces the non-interacting PDF,  $g^0(r)$ . On defining modified (short-ranged) direct-correlation functions:

$$\hat{c}_{ij}(r) = c_{ij}(r) + \beta\phi_{ij}(r) \quad (11)$$

we can express the LFF in a form where  $V_c(k)$  has been explicitly cancelled out.

$$G(k) = Tx[\hat{c}_{11} + \hat{c}_{12} + B_{11}(k) + B_{12}(k) - \hat{c}_{11}^0]/V_c(k). \quad (12)$$

This is free of numerical inaccuracies at small- $k$ , and contains the bridge terms that may be used to recover the compressibility sum rule etc. On the other hand, this requires explicit forms for the bridge functions (which can be constructed using the hard-disk model bridge function [6]). However, here we propose a much simpler, *practical*, approach based on using Eq. 4 which requires only the  $S(k)$  and  $S^0(k)$  which may be available from other sources beside the CHNC.

The 2-D compressibility sum rule [3] leads to the following small- $k$  form for the LFF.

$$G(k) = C_0 k \quad k \rightarrow 0 \quad (13)$$

$$C_0 = \frac{1}{\pi} + \frac{1}{4} \alpha r_s^2 \left[ \frac{\partial E_c}{\partial r_s} - r_s \frac{\partial^2 E_c}{\partial r_s^2} \right] \quad (14)$$

Here  $E_c$  is the correlation energy per particle in atomic units, and  $\alpha = 1/\sqrt{2}$ . Several fit formulae (based on QMC data, [19, 20, 21]) are available for  $E_c(r_s)$ . Hence  $C_0$  can be calculated easily. Equation 13 is valid only for small- $k$  where  $G(k)$  is linear in  $k$ . Based on more extensive calculations using Eq. 12, we assume a linear interpolation for the small- $k$  region  $k_1$  to  $k_c$ , where  $k_1$  is the smallest value of  $k$  in our  $S(k)$  tabulation. That is, we replace the form:

$$G(k) = 1 - \frac{T_{cf}}{nV_c(k)} \left[ \frac{1}{S(k)} - \frac{1}{S^0(k)} \right]; \quad \text{all } k \quad (15)$$

by the constrained form:

$$G(k_1) = C_0 k_1$$

$$G(k) = \left[ G(k_c) - G(k_1) \right] \frac{k - k_1}{k_c - k_1} \quad k < k_c. \quad (16a)$$

$$G(k) = 1 - \frac{T_{cf}}{nV_c(k)} \left[ \frac{1}{S(k)} - \frac{1}{S^0(k)} \right] \quad k > k_c. \quad (16b)$$

Here we choose  $k_c = 2k_F$ . In practice,  $k_c$  is chosen to be the  $k$ -point closest to  $2k_F$  in the  $S(k)$  tabulation which gives a continuous accord between the low- $k$  and high- $k$  regimes, and hence  $k_c/k_F$  may be, e.g., 1.9 or 2.1.

*Results.* We now consider the LFF for  $r_s = 1, 5, 10$  and 20 calculated using Eq. 4, and displayed in Fig. 1.

We have also displayed the 3DEG local-field factor for  $r_s = 1$  and 5. The 3D-LFF shows a weak maximum near  $2k_F$  and tends to  $1 - g(0)$  for large  $k$ . The QMC data (triangles) are extracted from Fig. 1 of ref.[13], and are not available for  $r_s=20$ . Note that these do not tend to the  $1 - g(0)$  but has a linear- $q$  dependence for asymptotically large  $-q$ , consistent with a zeroth-order Lindhard response. For  $r_s = 1$ , the thermal wavevector ( $k_{th}/k_F = 2.88$ ) is larger than  $2k_F$ . Hence the region where  $G(k)$  is linear in  $k$  may extend well beyond  $2k_F$ . However, we have retained a linearization up to  $2k_F$  which joins with the  $k > 2k_F$  behaviour given from CHNC. Also, the extended linearity in the QMC is partly due to its large- $q$  asymptotic behaviour. For  $r_s=5$  strong-coupling effects show up and a broad hump-like structure near  $k/k_F \sim 3$  is manifest. When we go to  $r_s = 10$  this behaviour is more pronounced, and sharpens even more for  $r_s=20$ . The required large- $k$  behaviour,  $G(k) \rightarrow 1 - g(0)$ , of the LFF is automatically satisfied by CHNC and hence we do not impose it. The difference between  $1/S(k)$  and  $1/S^0(k)$  required in Eq. 15 increases for strong coupling, and the direct method of calculating the LFF, using Eq. 4, instead of Eq. 12 becomes adequate. Thus we compare the LFF calculated without imposing the compressibility sum rule, and using  $S(k)$  from two different sources and different (but equivalent) formulations. For the cases  $r_s = 10$  and 20, we have given (dashed line) LFFs evaluated purely using the  $S(k)$  and  $S^0(k)$  derived from CHNC, and using Eq. 12. These include only the  $B_{12}$  bridge term. The linear form based on the compressibility sum rule *has not been* imposed. We also present the LFFs (solid lines with circles) obtained using the  $S(k)$  given in 1989 by Tanatar and Ceperely[19], together with the linearized forms (solid lines with squares) resulting from them. These results show that the maximum around  $3k_F$  is obtained irrespective of the method used, while the small- $k$  region is clearly sensitive to the numerical procedures used. More details about the CHNC method and on-line access to our codes may be obtained at our website[22].

*conclusion* Unusual features of the 2D-LFF not found in the 3D-case, and unexpected from perturbation theory, have been revealed via the CHNC method. These results seem to be in agreement with the limited QMC results currently available. They should stimulate further work on the important problem of the 2D response using non-perturbative methods.

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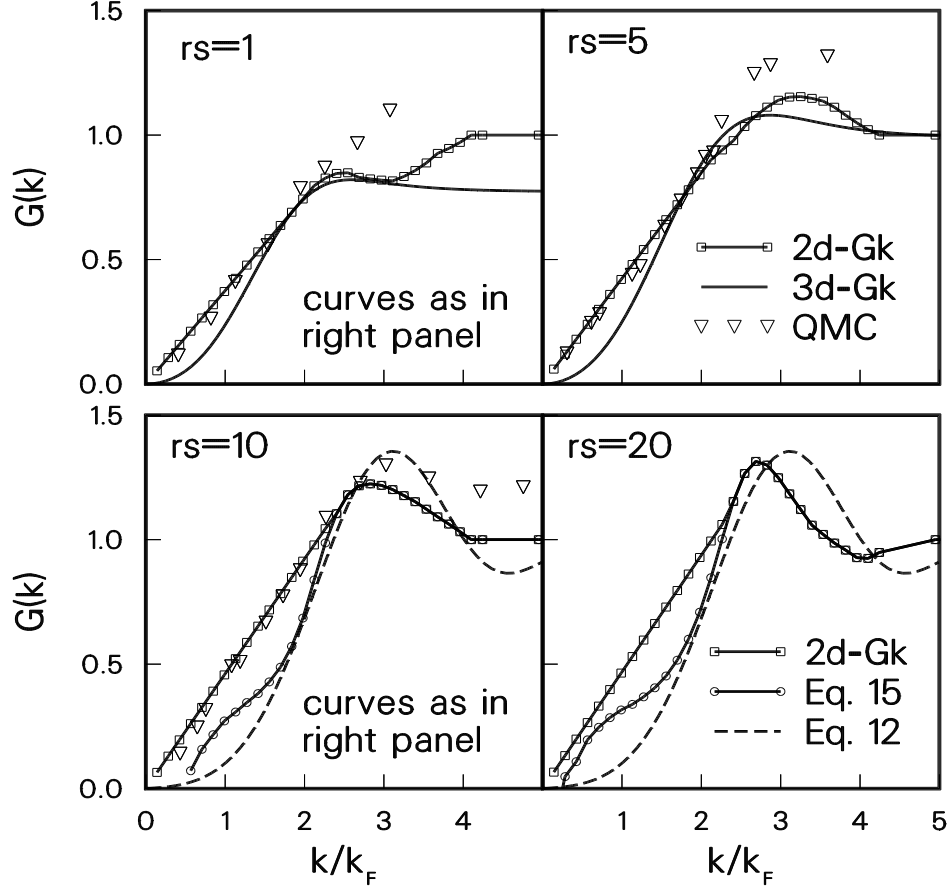


FIG. 1: The local-field factors calculated with linearization (squares), Eq. 16a, and without linearization (circles), Eq. 15, are shown for  $r_s=10$  and  $20$ . For  $r_s=1, 5$  and  $10$  QMC data (triangles) extracted from Fig. 1 of ref [13] are shown, and have a  $q$ -dependent asymptotic form, while CHNC tends to  $1 - g(0)$  for large  $q$ . The solid continuous line in the panels for  $r_s=1$  and  $5$  are the 3-D LFFs calculated from CHNC.

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